Introduction to Information Retrieval

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IIR 17: Hierarchical Clustering

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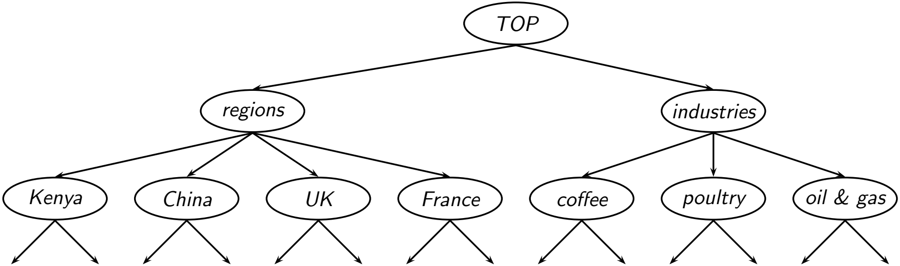
Outline

Hierarchical clustering

Our goal in hierarchical clustering is to create a hierarchy like the one we saw earlier in Reuters:



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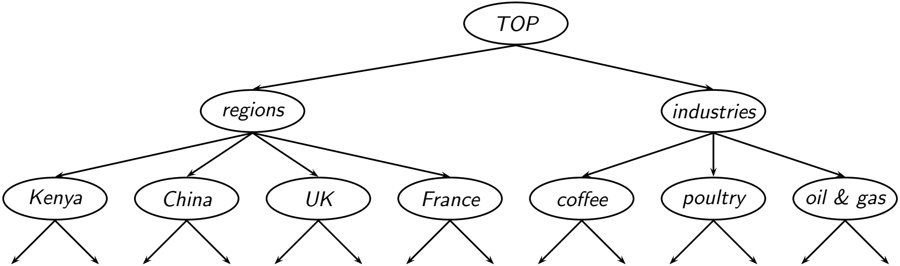

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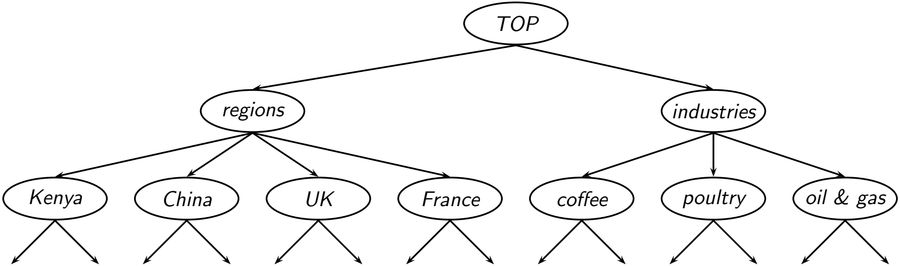

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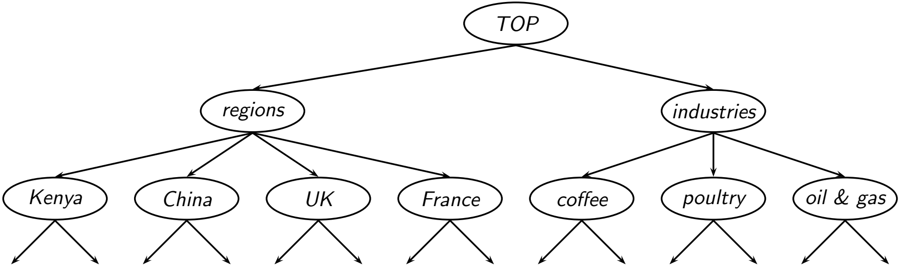


We want to create this hierarchy automatically.

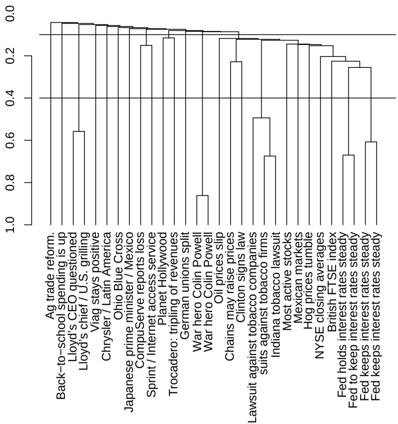
We can do this either top-down or bottom-up.

The best known bottom-up method is hierarchical agglomerative clustering.

Hierarchical agglomerative clustering (HAC)

- Assumes a similarity measure for determining the similarity of two clusters (up to now: similarity of documents).
- We will look at four different cluster similarity measures.
- Start with each document in a separate cluster
- Then repeatedly merge the two clusters that are most similar
- Until there is only one cluster
- The history of merging forms a binary tree or hierarchy.
- The standard way of depicting this history is a dendrogram.

A dendrogram



- The history of mergers can be read off from bottom to top.
- The horizontal line of each merger tells us what the similarity of the merger was.
- We can cut the dendrogram at a particular point (e.g., at 0.1 or 0.4) to get a flat clustering.

Divisive clustering

- Top-down (instead of bottom-up as in HAC)
- Start with all docs in one big cluster
- Then recursively split clusters
- Eventually each node forms a cluster on its own.
- $\rightarrow$ Bisecting K-means at the end

Naive HAC algorithm

$\textsc{SimpleHAC}(d_1, \ldots, d_N)$

for $n \leftarrow 1$ **to** N
do for $i \leftarrow 1$ **to** N
    do $C[n][i] \leftarrow \textsc{Sim}(d_n, d_i)$
    $I[n] \leftarrow 1$ *(keeps track of active clusters)*
$A \leftarrow []$ *(collects clustering as a sequence of merges)*
for $k \leftarrow 1$ **to** $N - 1$
do $\langle i, m \rangle \leftarrow \arg\max_{\{\langle i,m \rangle : i \neq m \wedge I[i]=1 \wedge I[m]=1\}} C[i][m]$
    $A.\textsc{Append}(\langle i, m \rangle)$ *(store merge)*
    for $j \leftarrow 1$ **to** N
    do $C[i][j] \leftarrow \textsc{Sim}(i, m, j)$
        $C[j][i] \leftarrow \textsc{Sim}(i, m, j)$
    $I[m] \leftarrow 0$ *(deactivate cluster)*
return A

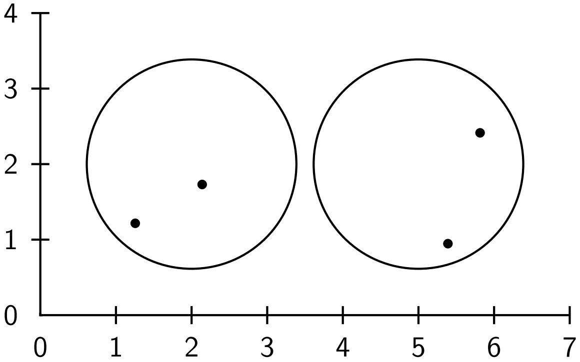
Computational complexity of the naive algorithm

- First, we compute the similarity of all $N \times N$ pairs of documents.
- Then, in each iteration:
  - We scan the $O(N \times N)$ similarities to find the maximum similarity.
  - We merge the two clusters with maximum similarity.
  - We compute the similarity of the new cluster with all other (surviving) clusters.
- There are $O(N)$ iterations, each performing a $O(N \times N)$ "scan" operation.
- Overall complexity is $O(N^3)$.
- We'll look at more efficient algorithms later.

Key question: How to define cluster similarity

- Single-link: Maximum similarity
  - Maximum over all document pairs
- Complete-link: Minimum similarity
  - Minimum over all document pairs
- Centroid: Average "intersimilarity"
  - Average over all document pairs
  - This is equivalent to the similarity of the centroids.
- Group-average: Average "intrasimilarity"
  - Average over all document pairs, including pairs of docs in the same cluster

Cluster similarity: Example



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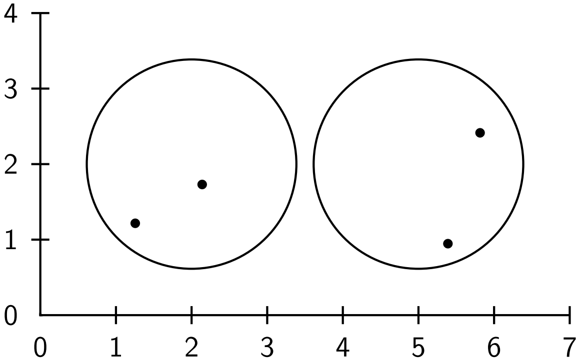

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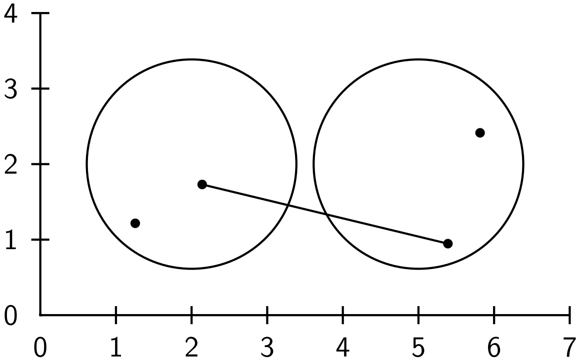

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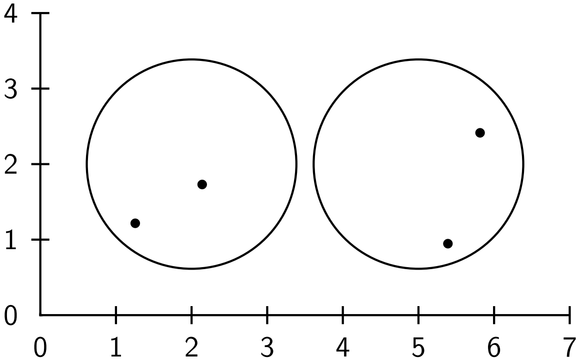

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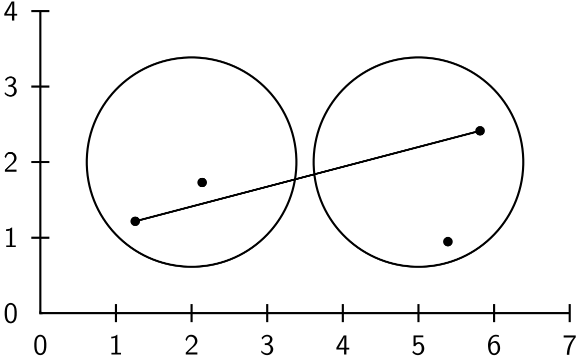
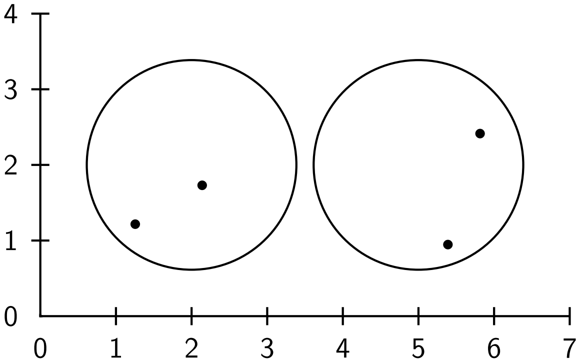


Centroid: Average intersimilarity

intersimilarity = similarity of two documents in different clusters



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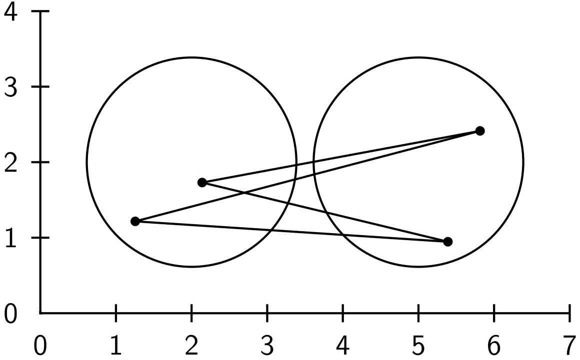

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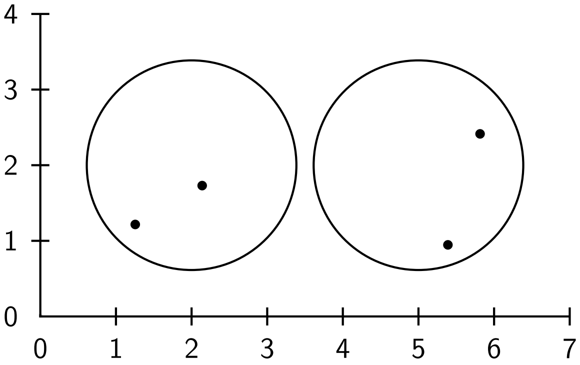

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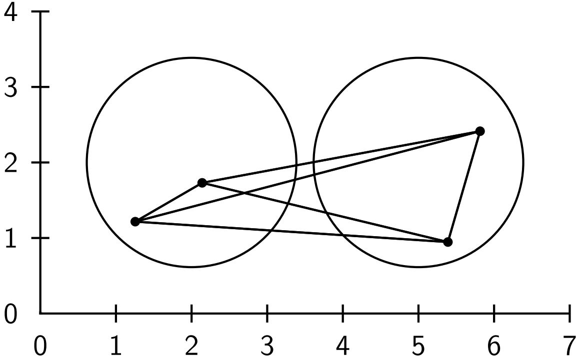
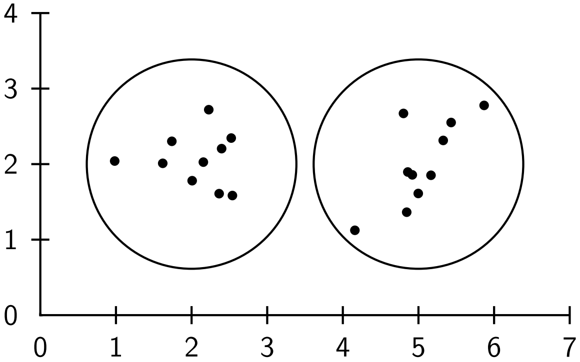


Cluster similarity: Larger example



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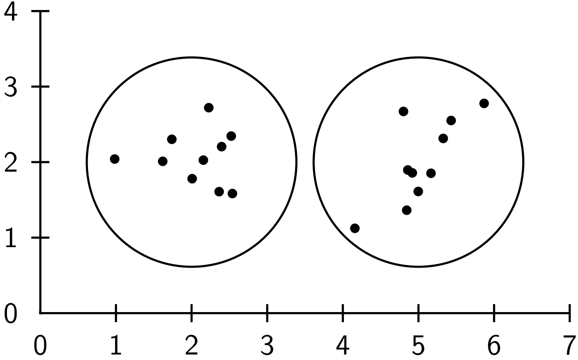

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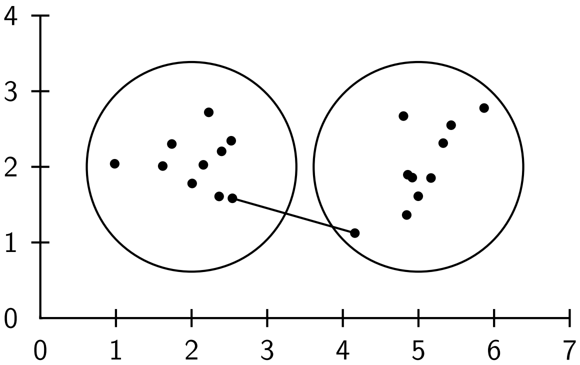

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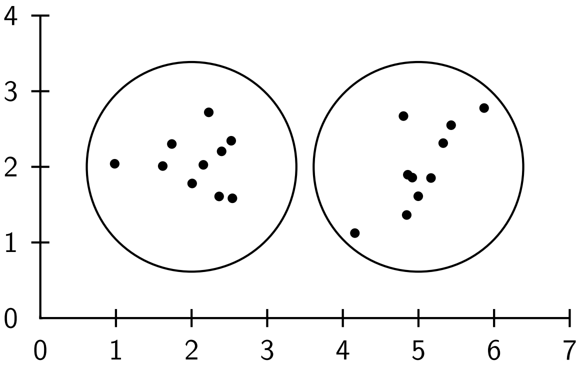

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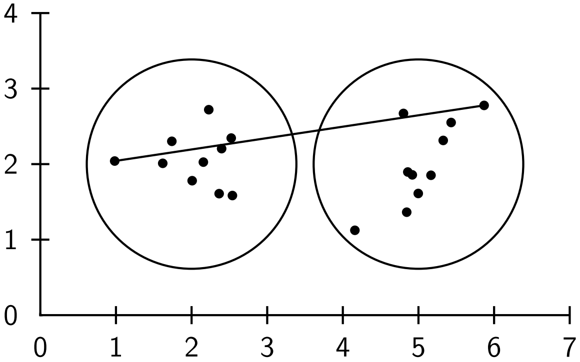

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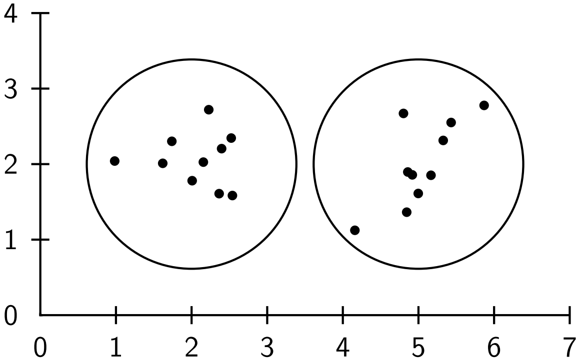

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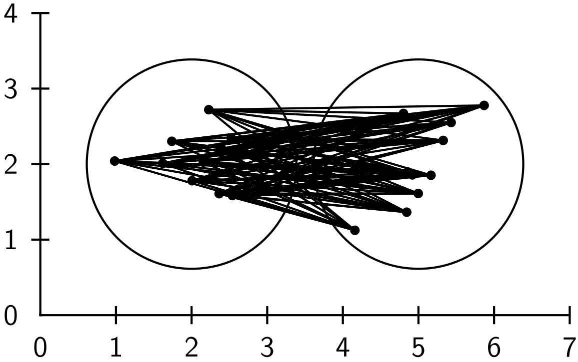

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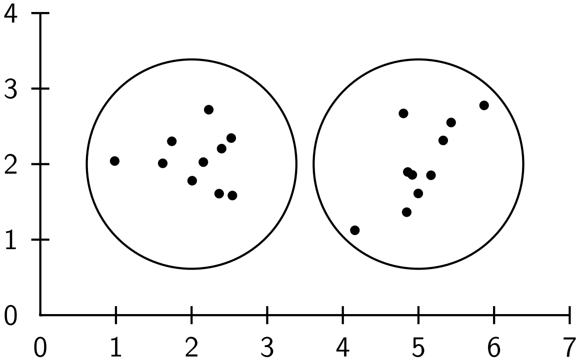

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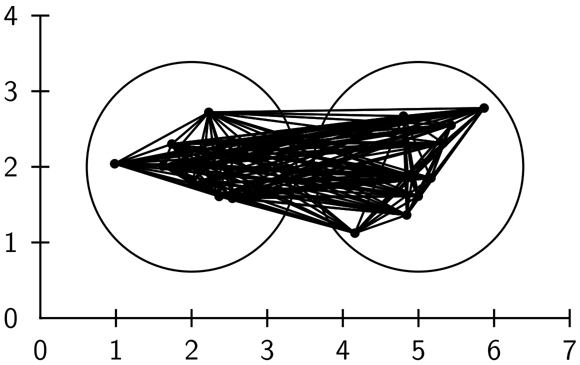

Outline

Single link HAC

- The similarity of two clusters is the maximum intersimilarity – the maximum similarity of a document from the first cluster and a document from the second cluster.
- Once we have merged two clusters, how do we update the similarity matrix?

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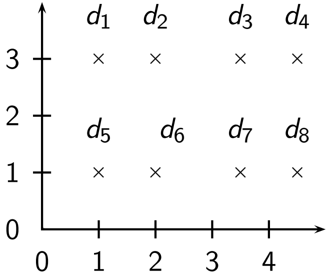
- The similarity of two clusters is the maximum intersimilarity – the maximum similarity of a document from the first cluster and a document from the second cluster.
- Once we have merged two clusters, how do we update the similarity matrix?
- This is simple for single link:

$$\text{SIM}(\omega_i, (\omega_{k_1} \cup \omega_{k_2})) = \max(\text{SIM}(\omega_i, \omega_{k_1}), \text{SIM}(\omega_i, \omega_{k_2}))$$

Single-link clustering: Example



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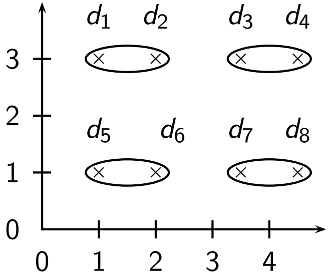

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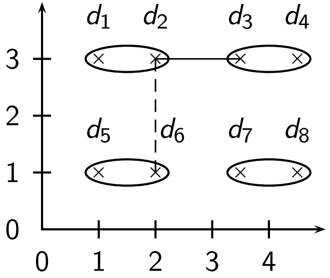

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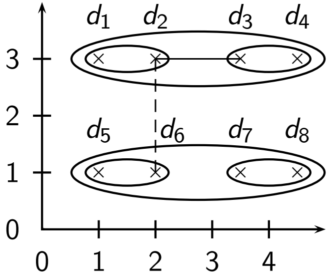
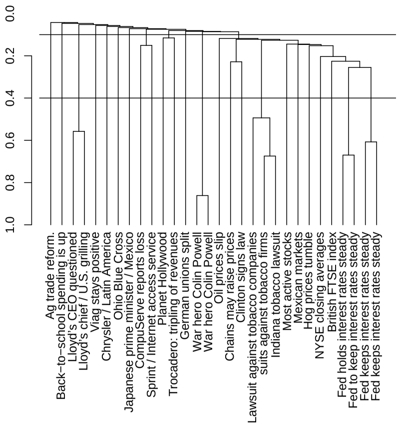
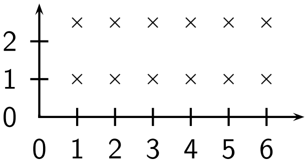


This dendrogram was produced by single-link

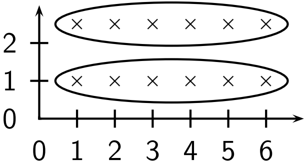


- Notice: many small clusters (1 or 2 members) being added to the main cluster
- There is no balanced 2-cluster or 3-cluster clustering that can be derived by cutting the dendrogram.

What cluster structure after 10 mergers?



Single-link: Chaining



Single-link clustering often produces long, straggly clusters. For most applications, these are undesirable.

Complete link HAC

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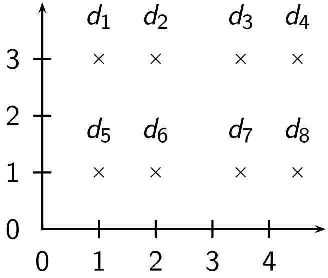
- Once we have merged two clusters, how do we update the similarity matrix?
- Again, this is simple:

$$\text{SIM}(\omega_i, (\omega_{k_1} \cup \omega_{k_2})) = \min(\text{SIM}(\omega_i, \omega_{k_1}), \text{SIM}(\omega_i, \omega_{k_2}))$$

- We measure the similarity of two clusters by computing the radius of the cluster that we would get if we merged them.

Complete link clustering: Example



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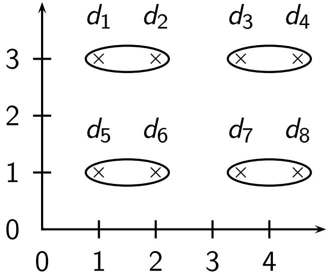

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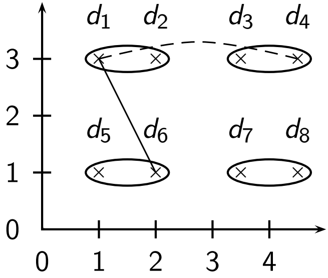

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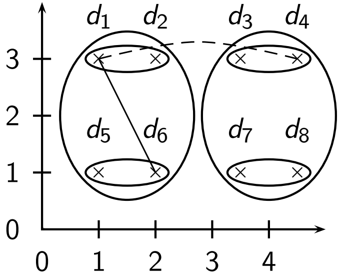
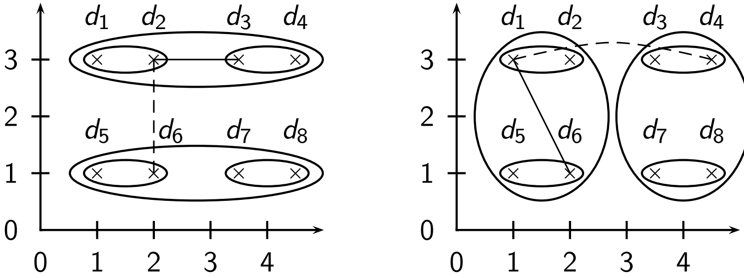
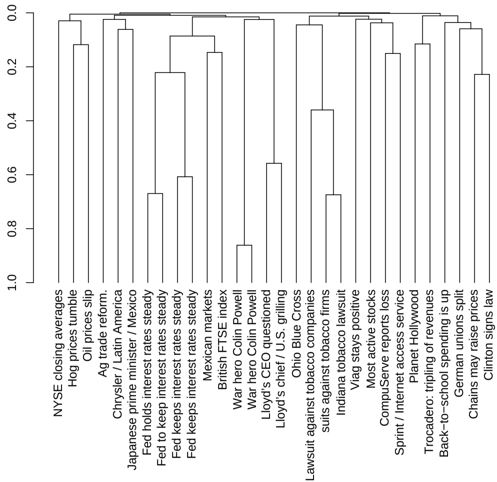


Single-link vs. Complete link clustering

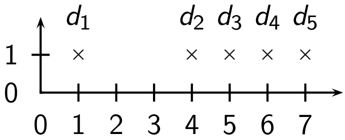


Complete-link dendrogram



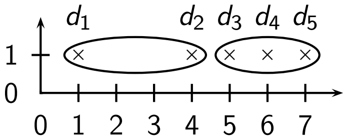
- Notice that this dendrogram is much more balanced than the single-link one.
- We can create a 2-cluster clustering with two clusters of about the same size.

Complete-link: Sensitivity to outliers



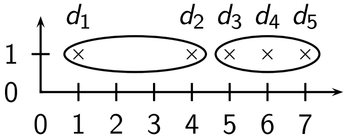
What is the intuitively best 2-cluster clustering here?

Complete-link: Sensitivity to outliers



The complete-link clustering of this set. It's not intuitive.

Complete-link: Sensitivity to outliers



The complete-link clustering of this set. It's not intuitive. This shows that a single outlier can have a large effect on the final outcome of complete-link clustering. Coordinates: $1 + 2 \times \epsilon, 4, 5 + 2 \times \epsilon, 6, 7 - \epsilon$.

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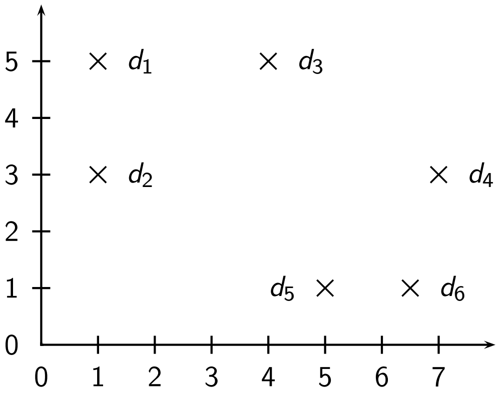
$$\text{SIM-CENT}(\omega_i, \omega_j) = \vec{\mu}(\omega_i) \cdot \vec{\mu}(\omega_j)$$

- Hence the name: centroid HAC
- Note: this is the dot product, not cosine similarity!

Centroid clustering: Example



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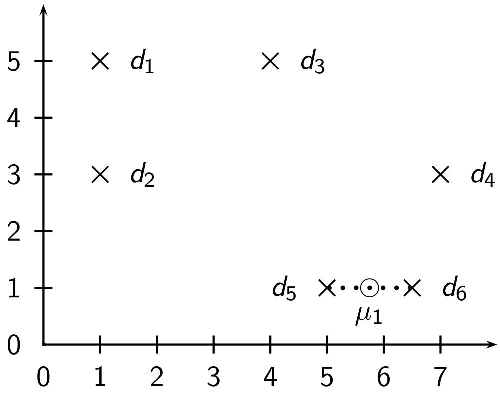

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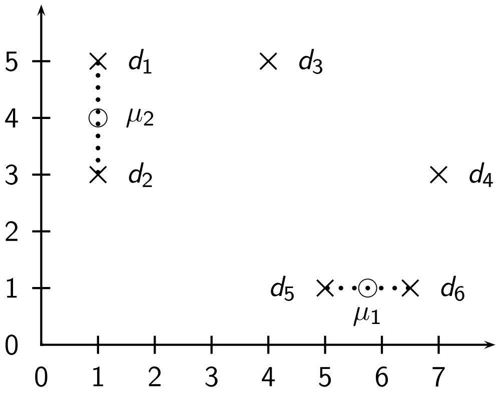

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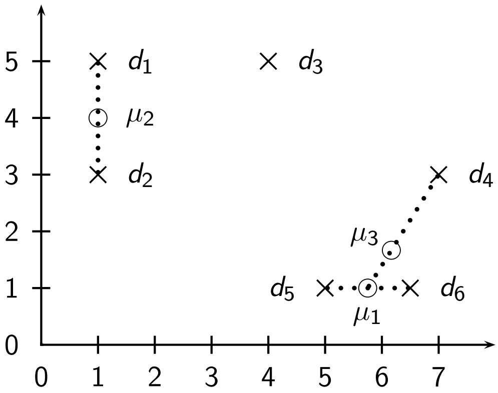
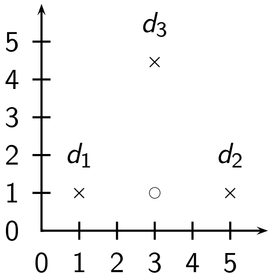
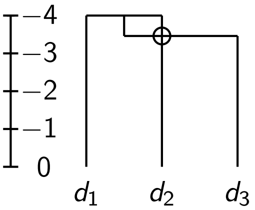


Inversion in centroid clustering

- In an inversion, the similarity increases during a merge sequence. Results in an "inverted" dendrogram.
- Below: Similarity of the first merger ($d_1 \cup d_2$) is -4.0, similarity of second merger ($(d_1 \cup d_2) \cup d_3$) is ≈ -3.5.





Inversions

- Hierarchical clustering algorithms that allow inversions are inferior.
- The rationale for hierarchical clustering is that at any given point, we've found the most coherent cluster of a given size.
- Intuitively: smaller clusters should be more coherent than larger clusters.
- An inversion contradicts this intuition: we have a large cluster that is more coherent than one of its subclusters.

Group-average agglomerative clustering (GAAC)

- GAAC also has an "average-similarity" criterion, but does not have inversions.
- The similarity of two clusters is the average intrasimilarity – the average similarity of all document pairs (including those from the same cluster).
- But we exclude self-similarities.

Group-average agglomerative clustering (GAAC)

- Again, the above definition is inefficient ($O(N^2)$) and there is an equivalent, more efficient, centroid-based definition:

$$\text{SIM-GA}(\omega_i, \omega_j) =$$

$$\frac{1}{(N_i + N_j)(N_i + N_j - 1)}[(\sum_{d_m \in \omega_i \cup \omega_j} \vec{d}_m)^2 - (N_i + N_j)]$$

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- However, we can only use GAAC for vector representations.
- For other types of document representations (or if only pairwise similarities for document are available): use complete-link.
- There are also some applications for single-link (e.g., duplicate detection in web search).

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- For high efficiency, use flat clustering (or perhaps bisecting *k*-means)
- For deterministic results: HAC
- When a hierarchical structure is desired: hierarchical algorithm
- HAC also can be applied if K cannot be predetermined (can start without knowing K)

Outline

Time complexity of HAC

- The single-link algorithm we just saw is $O(N^2)$.
- Much more efficient than the $O(N^3)$ algorithm we looked at earlier!
- There is no known $O(N^2)$ algorithm for complete-link, centroid and GAAC.
- Best time complexity for these three is $O(N^2 \log N)$: See book.
- In practice: little difference between $O(N^2 \log N)$ and $O(N^2)$.

Combination similarities of the four algorithms

clustering algorithm	$\text{sim}(\ell, k_1, k_2)$
single-link	$\max(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
complete-link	$\min(\text{sim}(\ell, k_1), \text{sim}(\ell, k_2))$
centroid	$(\frac{1}{N_m}\vec{v}_m) \cdot (\frac{1}{N_\ell}\vec{v}_\ell)$
group-average	$\frac{1}{(N_m+N_\ell)(N_m+N_\ell-1)}[(\vec{v}_m + \vec{v}_\ell)^2 - (N_m + N_\ell)]$

Comparison of HAC algorithms

method	combination similarity	time compl.	optimal?	comment
single-link	max intersimilarity of any 2 docs	$\Theta(N^2)$	yes	chaining effect
complete-link	min intersimilarity of any 2 docs	$\Theta(N^2 \log N)$	no	sensitive to outliers
group-average	average of all sims	$\Theta(N^2 \log N)$	no	best choice for most applications
centroid	average intersimilarity	$\Theta(N^2 \log N)$	no	inversions can occur

What to do with the hierarchy?

- Use as is (e.g., for browsing as in Yahoo hierarchy)
- Cut at a predetermined threshold
- Cut to get a predetermined number of clusters K
- Hierarchical clustering is often used to get K flat clusters. The hierarchy is then ignored.

Bisecting K-means: A top-down algorithm

- Start with all documents in one cluster
- Split the cluster into 2 using K-means
- Of the clusters produced so far, select one to split (e.g. select the largest one)
- Repeat until we have produced the desired number of clusters

Bisecting K-means

$\textsc{BisectingKMeans}(d_1, \ldots, d_N)$

$\omega_0 \leftarrow \{\vec{d}_1, \ldots, \vec{d}_N\}$

$\mathit{leaves} \leftarrow \{\omega_0\}$

for $k \leftarrow 1$ **to** $K - 1$

do $\omega_k \leftarrow \textsc{PickClusterFrom}(\mathit{leaves})$

$\quad \{\omega_i, \omega_j\} \leftarrow \textsc{KMeans}(\omega_k, 2)$

$\quad \mathit{leaves} \leftarrow \mathit{leaves} \setminus \{\omega_k\} \cup \{\omega_i, \omega_j\}$

return *leaves*

Bisecting K-means

- If we don't generate a complete hierarchy, then a top-down algorithm like bisecting K-means is much more efficient than HAC algorithms.

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- If we don't generate a complete hierarchy, then a top-down algorithm like bisecting K-means is much more efficient than HAC algorithms.
- But bisecting K-means is not deterministic.
- Why?

Outline

Major issue in clustering – labeling

- After a clustering algorithm finds a set of clusters: how can they be useful to the end user?
- We need a pithy label for each cluster.
- For example, in search result clustering for "jaguar": "animal", "car", "operating system"
- How can we do this?